

On graphs with maximum Harary spectral radius*

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Abstract

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The Harary matrix $RD(G)$ of G , which is initially called the reciprocal distance matrix, is an $n \times n$ matrix whose (i, j) -entry is equal to $\frac{1}{d_{ij}}$ if $i \neq j$ and 0 otherwise, where d_{ij} is the distance of v_i and v_j in G . In this paper, we characterize graphs with maximum spectral radius of Harary matrix in three classes of simple connected graphs with n vertices: graphs with fixed matching number, bipartite graphs with fixed matching number, and graphs with given number of cut edges, respectively.

Keywords: Harary matrix, Harary spectral radius, matching number, cut edge.

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1 Introduction

In this paper we are concerned with simple finite graphs. Undefined notation and terminology can be found in [1]. Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Let $N_G(v)$ be the neighborhood of the vertex v of G , and d_{ij} be the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G .

The Harary matrix $RD(G)$ of G , which is initially called the reciprocal distance matrix, is an $n \times n$ matrix (RD_{ij}) such that

$$RD_{ij} = \begin{cases} \frac{1}{d_{ij}} & \text{if } i \neq j, \\ 0 & \text{otherwise.} \end{cases}$$

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As we know, in many instances the distant atoms influence each other much less than near atoms. Harary matrix was introduced by Ivanciuc et al.[9] as an important molecular matrix to research this interaction, and it was also successfully used in a study concerning computer generation of acyclic graphs based on local vertex invariants and topological indices. Moreover, It is shown that the Harary spectral radius is able to produce fair QSPR models for the boiling points, molar heat capacities, vaporization enthalpies, refractive indices and densities for C_6 - C_{10} alkanes.

Ivanciuc et al. [10] proposes to use the maximum eigenvalues of distance-based matrices as structural descriptors. The lower and upper bounds of the maximum eigenvalues of Harary matrix, and the Nordhaus-Gaddum-type results for it were obtained in [3, 16]. Mathematical properties and applications of Harary index are reported in [4, 6, 7, 12–15]. Some lower and upper bounds for Harary energy of connected (n, m) -graphs were obtain in [8].

A matching in a graph is a set of pairwise nonadjacent edges. A maximum matching is one which covers as many vertices as possible. The number of edges in a maximum matching of a graph G is called the matching number of G and denoted by $\alpha'(G)$. In this paper we characterize graphs with maximum spectral radius of Harary matrix in three classes of simple connected graphs with n vertices: graphs with fixed matching number, bipartite graphs with fixed matching number, and graphs with given number of cut edges, respectively.

2 Preliminaries

Since RD is a real symmetric matrix, its eigenvalues are all real. Let $\rho(G)$ be the spectral radius of $RD(G)$, called Harary spectral radius. By the Perron-Frobenius theorem, the Harary spectral radius of a connected graph G corresponds to a unique positive unit eigenvector $X = (x_1, x_2, \dots, x_n)^T$, called principal eigenvector of $RD(G)$. Then

$$\rho(G)x_i = \sum_{j \neq i} \frac{1}{d_{ij}} x_j. \quad (1)$$

The following lemma is an immediate consequence of Perron-Frobenius Theorem.

Lemma 2.1. *Let G be a connected graph with $u, v \in V(G)$ and $uv \notin E(G)$. Then $\rho(G) < \rho(G + uv)$.*

Let G be a connected graph, and H a subgraph of G . We know that H can be obtained from G by deleting edges, and possibly vertices.

Corollary 2.2. *If H is a subgraph of a connected graph G , then $\rho(H) < \rho(G)$.*

Lemma 2.3. *Let G be a connected graph with $v_r, v_s \in V(G)$. If $N_G(v_r) \setminus \{v_s\} = N_G(v_s) \setminus \{v_r\}$, then $x_r = x_s$.*

Proof. From Eq. (1), we know that

$$\rho(G)x_r = \sum_{j \neq r} \frac{1}{d_{rj}}x_j = \frac{1}{d_{rs}}x_s + \sum_{j \neq s, r} \frac{1}{d_{rj}}x_j,$$

and,

$$\rho(G)x_s = \sum_{j \neq s} \frac{1}{d_{sj}}x_j = \frac{1}{d_{sr}}x_r + \sum_{j \neq s, r} \frac{1}{d_{sj}}x_j.$$

Since $N_G(v_r) \setminus \{v_s\} = N_G(v_s) \setminus \{v_r\}$, we have that $d_{rj} = d_{sj}$ for $j \neq s, r$. Then

$$\rho(G)(x_r - x_s) = -\frac{1}{d_{sr}}(x_r - x_s),$$

and thus $x_r = x_s$. □

3 Graphs with given matching number

Let $G_1 \cup \dots \cup G_k$ be the vertex-disjoint union of the graphs G_1, \dots, G_k ($k \geq 2$), and $G_1 \vee G_2$ be the graph obtained from $G_1 \cup G_2$ by joining each vertex of G_1 to each vertex of G_2 .

Lemma 3.1. *Let $G_1 = K_s \vee (K_{n_1} \cup K_{n_2} \cup \dots \cup K_{n_k})$ and $G_2 = K_s \vee (K_{n_1-1} \cup K_{n_2+1} \cup \dots \cup K_{n_k})$. If $n_2 \geq n_1 \geq 2$, then $\rho(G_1) < \rho(G_2)$.*

Proof. Let $\rho(G_1)$ be the Harary spectral radius of G_1 and X the corresponding principal eigenvector. By Lemma 2.3, X can be written as

$$X = (\underbrace{y_1, \dots, y_1}_{n_1}, \underbrace{y_2, \dots, y_2}_{n_2}, \dots, \underbrace{y_k, \dots, y_k}_{n_k}, \underbrace{y_0, \dots, y_0}_s).$$

From Eq. (1), we have

$$\begin{aligned} \rho(G_1)y_1 &= (n_1 - 1)y_1 + \frac{1}{2}n_2y_2 + \sum_{i=3}^k \frac{1}{2}n_iy_i + sy_0, \\ \rho(G_1)y_2 &= \frac{1}{2}n_1y_1 + (n_2 - 1)y_2 + \sum_{i=3}^k \frac{1}{2}n_iy_i + sy_0. \end{aligned}$$

It implies that

$$\rho(G_1)(y_1 - y_2) = \frac{1}{2}n_1y_1 - y_1 - \frac{1}{2}n_2y_2 + y_2,$$

that is,

$$(\rho(G_1) + 1 - \frac{1}{2}n_1)y_1 = (\rho(G_1) + 1 - \frac{1}{2}n_2)y_2.$$

Note that K_{s+n_2} is a subgraph of G_1 and $n_2 \geq n_1$, we have that

$$\rho(G_1) > \rho(K_{s+n_2}) = s + n_2 - 1 \geq n_2.$$

Then we have that

$$y_1 \leq y_2.$$

From the definition of Harary matrix, we know that

$$RD(G_1) = \begin{pmatrix} (J - I)_{n_1 \times n_1} & \frac{1}{2}J_{n_1 \times n_2} & \cdots & \frac{1}{2}J_{n_1 \times n_k} & J_{n_1 \times s} \\ \frac{1}{2}J_{n_2 \times n_1} & (J - I)_{n_2 \times n_2} & \cdots & \frac{1}{2}J_{n_2 \times n_k} & J_{n_2 \times s} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{2}J_{n_k \times n_1} & J_{n_k \times n_2} & \cdots & (J - I)_{n_k \times n_k} & J_{n_k \times s} \\ J_{s \times n_1} & J_{s \times n_2} & \cdots & J_{s \times n_k} & (J - I)_{s \times s} \end{pmatrix},$$

and,

$$RD(G_2) = \begin{pmatrix} (J - I)_{(n_1-1) \times (n_1-1)} & \frac{1}{2}J_{(n_1-1) \times (n_2+1)} & \cdots & \frac{1}{2}J_{(n_1-1) \times n_k} & J_{(n_1-1) \times s} \\ \frac{1}{2}J_{(n_2+1) \times (n_1-1)} & (J - I)_{(n_2+1) \times (n_2+1)} & \cdots & \frac{1}{2}J_{(n_2+1) \times n_k} & J_{n_2 \times s} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{2}J_{n_k \times (n_1-1)} & J_{n_k \times (n_2+1)} & \cdots & (J - I)_{n_k \times n_k} & J_{n_k \times s} \\ J_{s \times (n_1-1)} & J_{s \times (n_2+1)} & \cdots & J_{s \times n_k} & (J - I)_{s \times s} \end{pmatrix}.$$

Thus

$$RD(G_2) - RD(G_1) = \begin{pmatrix} 0_{(n_1-1) \times (n_1-1)} & -\frac{1}{2}J_{(n_1-1) \times 1} & 0_{(n_1-1) \times n_2} & 0 \\ -\frac{1}{2}J_{1 \times (n_1-1)} & 0_{1 \times 1} & \frac{1}{2}J_{1 \times n_2} & 0 \\ 0_{n_2 \times (n_1-1)} & \frac{1}{2}J_{n_2 \times 1} & 0_{n_2 \times n_2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Hence

$$\begin{aligned} \rho(G_2) - \rho(G_1) &\geq X^T RD(G_2)X - X^T RD(G_1)X \\ &= X^T (RD(G_2) - RD(G_1))X = n_2y_1y_2 - (n_1 - 1)y_1^2 \\ &> 0. \end{aligned}$$

We complete the proof. \square

Lemma 3.2. Let $G = K_s \vee (\overline{K_{k-1}} \cup K_{2t+1})$ with $t \geq 1, k \geq 3$, and $G' = K_{s+t} \vee \overline{K_{k+t}}$. One has that $\rho(G) < \rho(G')$.

Proof. Let $\rho = \rho(G)$ be the Harary spectral radius of G and X be the principal eigenvector. By Lemma 2.3, X is positive and can be written as

$$X = (\underbrace{x, \dots, x}_s, \underbrace{y, \dots, y}_{k-1}, \underbrace{z, \dots, z}_{2t+1})^T.$$

From the definition of Harary matrix, we know that

$$RD(G) = \begin{pmatrix} (J - I)_{s \times s} & J_{s \times (k-1)} & J_{s \times (2t+1)} \\ J_{(k-1) \times s} & \frac{1}{2}(J - I)_{(k-1) \times (k-1)} & \frac{1}{2}J_{(k-1) \times (2t+1)} \\ J_{(2t+1) \times s} & \frac{1}{2}J_{(2t+1) \times (k-1)} & (J - I)_{(2t+1) \times (2t+1)} \end{pmatrix}$$

and

$$RD(G') = \begin{pmatrix} (J - I)_{s \times s} & J_{s \times (k-1)} & J_{s \times t} & J_{s \times t} & J_{s \times 1} \\ J_{(k-1) \times s} & \frac{1}{2}(J - I)_{(k-1) \times (k-1)} & J_{(k-1) \times t} & \frac{1}{2}J_{(k-1) \times t} & \frac{1}{2}J_{(k-1) \times 1} \\ J_{t \times s} & J_{t \times (k-1)} & (J - I)_{t \times t} & J_{t \times t} & J_{t \times 1} \\ J_{t \times s} & \frac{1}{2}J_{t \times (k-1)} & J_{t \times t} & \frac{1}{2}(J - I)_{t \times t} & \frac{1}{2}J_{t \times 1} \\ J_{1 \times s} & \frac{1}{2}J_{1 \times (k-1)} & J_{1 \times t} & \frac{1}{2}J_{1 \times t} & 0_{1 \times 1} \end{pmatrix},$$

thus

$$\begin{aligned} \rho(G') - \rho &\geq X^T(RD(G') - RD(G))X \\ &= t(k-1)yz - tz^2 \\ &= tz((k-1)y - z). \end{aligned} \tag{2}$$

As X is the principal eigenvector corresponding to $\rho = \rho(G)$, from Eq. (1), we have

$$\begin{aligned} \rho y &= sx + \frac{k-2}{2}y + \frac{1}{2}(2t+1)z, \\ \rho z &= sx + \frac{k-1}{2}y + 2tz. \end{aligned}$$

Then

$$\frac{y}{z} = \frac{2\rho - 2t + 1}{2\rho + 1}. \tag{3}$$

Hence

$$\begin{aligned} (k-1)y - z &= (k-1)\frac{2\rho - 2t + 1}{2\rho + 1}z - z \\ &= \frac{z}{2\rho + 1}(2(k-2)\rho - (k-1)(2t-1) - 1) \\ &= \frac{2(k-2)z}{2\rho + 1}\left(\rho - \frac{(k-1)(2t-1) + 1}{2(k-2)}\right) \\ &> \frac{2(k-2)z}{2\rho + 1}(\rho - 2t). \end{aligned}$$

Note that K_{s+2t+1} is a subgraph of G , by Corollary 2.2, we have that

$$\rho > \rho(K_{s+2t+1}) = s + 2t > 2t.$$

Hence we have that

$$\rho(G') - \rho > tz \frac{2(k-2)z}{2\rho+1}(\rho - 2t) > 0.$$

We complete the proof. \square

A component of a graph G is said to be even (odd) if it has an even (odd) number of vertices. We use $o(G)$ to denote the number of odd components of G . Let G be a graph on n vertices with $\alpha'(G) = p$. By the Tutte-Berge formula,

$$n - 2p = \max\{o(G - X) - |X| : X \subset V(G)\}.$$

Theorem 3.3. *Let G be a graph on n vertices with $\alpha'(G) = p$ which has the maximum Harary spectral radius. Then we have that*

1. if $p = \lfloor \frac{n}{2} \rfloor$, then $G = K_n$;
2. if $1 \leq p < \lfloor \frac{n}{2} \rfloor$, then $G = K_p \vee \overline{K_{n-p}}$.

Proof. The first assertion is trivial, and so we only need to prove the second assertion. Let X_0 be a vertex subset such that $n - 2p = o(G - X_0) - |X_0|$. For convenience, let $|X_0| = s$ and $o(G - X_0) = k$. Then $n - 2p = k - s$. Since $1 \leq p < \lfloor \frac{n}{2} \rfloor$, we know that $k - s \geq 2$. Hence $k \geq 3$.

If $G - X_0$ has an even component, then by adding an edge to G between a vertex of an even component and a vertex of an odd component of $G - X_0$, we obtain a graph G' with matching number p . From Lemma 2.1, we know that $\rho(G') > \rho(G)$, a contradiction to the assumption that G has the maximum Harary spectral radius. So we know that all the components of $G - X_0$ are odd. Let G_1, G_2, \dots, G_k be the odd components of $G - X_0$. Similarly, G_1, G_2, \dots, G_k and the subgraph induced by X_0 are all complete, and every vertex of G_i ($i = 1, \dots, k$) is adjacent to every vertex in X_0 . Thus $G = K_s \vee (K_{n_1} \cup K_{n_2} \cup \dots \cup K_{n_k})$, where $n_i = |V(G_i)|$ for $i = 1, 2, \dots, k$.

First, we claim that $G - X_0$ has at most one odd component whose number of vertex is more than one. Assume without loss of generality that $n_2 \geq n_1 \geq 3$. Let $G' = K_s \vee (K_{n_1-2} \cup K_{n_2+2} \cup \dots \cup K_{n_k})$. We can easily checked that $\alpha(G') = p$. From Lemma 3.1, we know that $\rho(G) < \rho(G')$, a contradiction. Then $G = K_s \vee (\overline{K_{k-1}} \cup K_t)$, where $s + t + k - 1 = n$. By Lemma 3.2, we know that $t = 1$. The result follows. \square

4 Bipartite graphs with given matching number

Lemma 4.1 ([2]). *Let K_{n_1, n_2} be a completed bipartite graph with $n = n_1 + n_2$ vertices. One has that*

$$\rho(K_{n_1, n_2}) = \frac{1}{4}(n - 2 + \sqrt{n^2 + 12n_1n_2}).$$

Corollary 4.2.

$$\rho(K_{1, n-1}) < \rho(K_{2, n-2}) < \dots < \rho(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}). \quad (4)$$

A covering of a graph G is a vertex subset $K \subseteq V(G)$ such that each edge of G has at least one end in the set K . The number of vertices in a minimum covering of a graph G is called the covering number of G and denoted by $\beta(G)$.

Lemma 4.3. (The König-Egerváry Theorem, [5, 11]). *In any bipartite graph, the number of edges in a maximum matching is equal to the number of vertices in a minimum covering.*

Let $G = G[X, Y] \neq K_{p, n-p}$ be a bipartite graph such that $\alpha'(G) = p$. From Lemma 4.3, we know that $\beta(G) = p$. Let S be a minimum covering of G and $X_1 = S \cap X \neq \emptyset$, $Y_1 = S \cap Y \neq \emptyset$. Set $X_2 = X \setminus X_1$, $Y_2 = Y \setminus Y_1$. We have that $E(X_2, Y_2) = \emptyset$ since S is a covering of G .

Let $G^*[X, Y]$ be a bipartite graph with the same vertex set as G such that $E(G^*) = \{xy : x \in X_1, y \in Y\} \cup \{xy : x \in X_2, y \in Y_1\}$. Obviously, G is a subgraph of G^* . From Lemma 2.1, we know that

$$\rho(G) \leq \rho(G^*), \quad (5)$$

with equality holds if and only if $G = G^*$.

Let

$$G' = G^* - \{uv : u \in X_2, v \in Y_1\} + \{uw : u \in X_2, w \in X_1\},$$

and

$$G'' = G^* - \{uv : u \in X_1, v \in Y_2\} + \{uw : u \in Y_2, w \in Y_1\}.$$

Then we have the following conclusion:

Lemma 4.4. *Let G^*, G' and G'' be the graph defined above (see Figure 1) with $X_2 \neq \emptyset$ and $Y_2 \neq \emptyset$. Then one has*

$$\rho(G^*) < \rho(G'), \quad \text{or} \quad \rho(G^*) < \rho(G''). \quad (6)$$

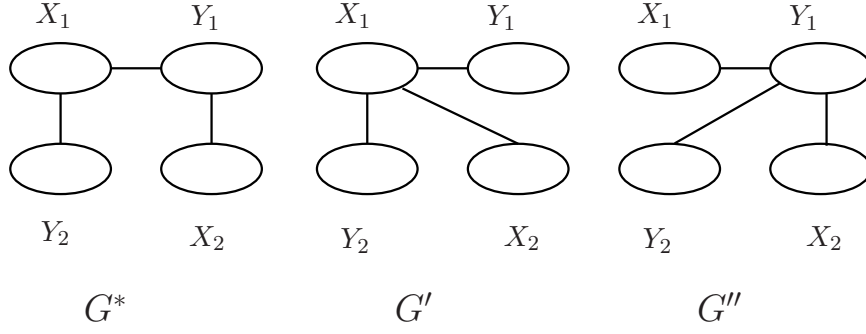


Figure 1. G^* , G' and G''

Proof. Let $\rho = \rho(G^*)$ be the Harary spectral radius of G^* and X the principal eigenvector. By Lemma 2.3, X is positive and can be written as

$$X = (\underbrace{x_1, \dots, x_1}_a, \underbrace{x_2, \dots, x_2}_b, \underbrace{y_1, \dots, y_1}_c, \underbrace{y_2, \dots, y_2}_d)^T,$$

where $a = |X_1|, b = |X_2|, c = |Y_1|$ and $d = |Y_2|$.

As

$$RD(G^*) = \frac{1}{2}(J - I) + \begin{pmatrix} 0_{a \times a} & \frac{1}{2}J_{a \times b} & J_{a \times c} & J_{a \times d} \\ \frac{1}{2}J_{b \times a} & 0_{b \times b} & J_{b \times c} & \frac{1}{3}J_{b \times d} \\ J_{c \times a} & J_{c \times b} & 0_{c \times c} & \frac{1}{2}J_{c \times d} \\ J_{d \times a} & \frac{1}{3}J_{d \times b} & \frac{1}{2}J_{d \times c} & 0_{d \times d} \end{pmatrix}$$

and

$$RD(G') = \frac{1}{2}(J - I) + \begin{pmatrix} 0_{a \times a} & J_{a \times b} & J_{a \times c} & J_{a \times d} \\ J_{b \times a} & 0_{b \times b} & \frac{1}{2}J_{b \times c} & \frac{1}{2}J_{b \times d} \\ J_{c \times a} & \frac{1}{2}J_{c \times b} & 0_{c \times c} & \frac{1}{2}J_{c \times d} \\ J_{d \times a} & \frac{1}{2}J_{d \times b} & \frac{1}{2}J_{d \times c} & 0_{d \times d} \end{pmatrix},$$

we have

$$\begin{aligned} & X^T(RD(G') - RD(G^*))X \\ &= X^T \begin{pmatrix} 0_{a \times a} & \frac{1}{2}J_{a \times b} & 0_{a \times c} & 0_{a \times d} \\ \frac{1}{2}J_{b \times a} & 0_{b \times b} & -\frac{1}{2}J_{b \times c} & \frac{1}{6}J_{b \times d} \\ 0_{c \times a} & -\frac{1}{2}J_{c \times b} & 0_{c \times c} & 0_{c \times d} \\ 0_{d \times a} & \frac{1}{6}J_{d \times b} & 0_{d \times c} & 0_{d \times d} \end{pmatrix} X \\ &= abx_1x_2 - bcx_2y_1 + \frac{1}{3}bdx_2y_2 \\ &= bx_2(ax_1 - cy_1) + \frac{1}{3}bdx_2y_2. \end{aligned} \tag{7}$$

Similarly, one has that

$$X^T(RD(G'') - RD(G^*))X = dy_2(cy_1 - ax_1) + \frac{1}{3}bdx_2y_2.$$

It is easy to see that either $X^T(RD(G') - RD(G^*))X > 0$ or $X^T(RD(G'') - RD(G^*))X > 0$, i.e., $\rho(G^*) < \rho(G')$ or $\rho(G^*) < \rho(G'')$. This completes the proof. \square

By (5) and (6), together with Corollary 4.2, it is straightforward to see that

Theorem 4.5. *For any bipartite graph G with matching number p and $G \neq K_{p,n-p}$, one has that $\rho(G) < \rho(K_{p,n-p})$.*

5 Graphs with given number of cut edges

Lemma 5.1. *Let G be a graph with a cut edge $e = w_1w_2$, and G' be the graph obtained from G by contracting edge e and adding a pendent edge attaching at the contracting vertex (see Figure 2). If $d_G(w_i) \geq 2$ for $i = 1, 2$, we have that $\rho(G') > \rho(G)$.*

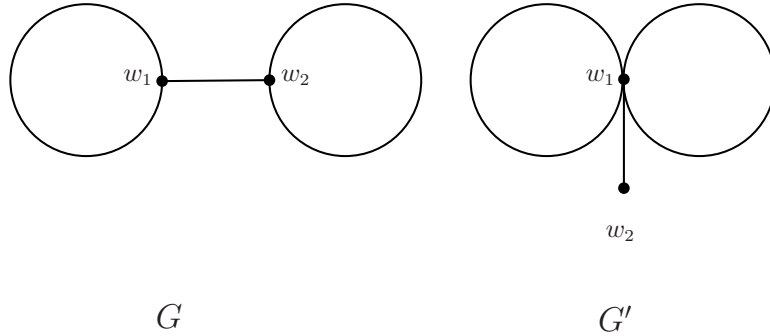


Figure 2. G and G'

Proof. Let $\rho(G)$ be the Harary spectral radius of G and X the corresponding principal eigenvector. Without loss of generality, we assume that $x_{w_1} \geq x_{w_2}$. We denote the contracting vertex by w_1 , and the pendant edge by w_1w_2 . Let G_i be the component of $G - e$ that contains w_i for $i = 1, 2$. Let $V'_1 = V(G_1) \setminus \{w_1\}$ and $V'_2 = V(G_2) \setminus \{w_2\}$. For any two vertices u and v , we have that

$$d_{G'}(u, v) = \begin{cases} d_G(u, v) - 1, & \text{if } u \in V(G_1) \text{ and } v \in V'_2, \\ d_G(u, v) + 1, & \text{if } u = w_2 \text{ and } v \in V'_2, \\ d_G(u, v), & \text{otherwise.} \end{cases}$$

Let

$$A = \sum_{w_1 \in V'_1, w_2 \in V'_2} \left(\frac{1}{d_{G'}(w_1, w_2)} - \frac{1}{d_G(w_1, w_2)} \right) x_{w_1} x_{w_2} > 0.$$

From the definition of Harary matrix, we know that

$$\begin{aligned} \rho(G') - \rho(G) &\geq X^T R D(G') X - X^T R D(G) X \\ &= \sum_{u, v \in V(G)} \left(\frac{1}{d_{G'}(u, v)} - \frac{1}{d_G(u, v)} \right) x_u x_v \\ &= 2A + 2 \sum_{u=w_1, v \in V'_2} \left(\frac{1}{d_{G'}(u, v)} - \frac{1}{d_G(u, v)} \right) x_u x_v \\ &\quad + 2 \sum_{u=w_2, v \in V'_2} \left(\frac{1}{d_{G'}(u, v)} - \frac{1}{d_G(u, v)} \right) x_u x_v \\ &= 2A + 2x_{w_1} \sum_{v \in V'_2} \left(\frac{x_{w_1}}{d_G(w_1, v)(d_G(w_1, v) - 1)} - \frac{x_{w_2}}{d_G(w_2, v)(d_G(w_2, v) + 1)} \right) \\ &= 2A + 2(x_{w_1} - x_{w_2})x_v \sum_{v \in V'_2} \frac{1}{d_G(w_1, v)(d_G(w_1, v) - 1)} \\ &\geq 2A > 0. \end{aligned}$$

Note that the last equality holds since $d_G(w_1, v) = d_G(w_2, v) + 1$ for any $v \in V'_2$. Hence we have our conclusion. \square

Assume that r_1, r_2, \dots, r_s are positive integers, and $s \leq t$. Let $K_t(r_1, r_2, \dots, r_s)$ be the graph that is obtained from K_t with $V(K_t) = \{v_1, v_2, \dots, v_t\}$ by attaching r_i pendant edges to vertex v_i for $1 \leq i \leq s$.

Lemma 5.2. *Let $G = K_t(r_1, r_2, \dots, r_s)$ and $G' = K_t(r_1 + r_2 + \dots + r_s)$. Then $\rho(G') > \rho(G)$.*

Proof. Let $\rho(G)$ be the Harary spectral radius of G and X the corresponding principal eigenvector. Let R_i be set of pendant vertices that is adjacent to v_i in G . From Lemma 2.3, we can suppose that $x_u = a_i$ for all $u \in R_i$ ($1 \leq i \leq s$). Without loss of generality, assume that $x_{v_1} \geq x_{v_i}$ for $2 \leq i \leq s$. Let $G'' = G - \{v_2 w : w \in R_2\} + \{v_1 w : w \in R_2\}$, that is, $G'' = K_t(r_1 + r_2, r_3, \dots, r_s)$. For any two vertices u and v , if neither u nor v belongs to R_2 , we know that $d_G(u, v) = d_{G''}(u, v)$; If both u and v belong to R_2 , we can also get $d_G(u, v) = d_{G''}(u, v)$. If exactly one of u and v belongs to R_2 , say $u \in R_2$, we have the following equation.

$$d_{G''}(u, v) = \begin{cases} d_G(u, v) - 1 = 2, & \text{if } v \in R_1, \\ d_G(u, v) - 1 = 1, & \text{if } v = v_1 \\ d_G(u, v) + 1 = 2, & \text{if } v = v_2, \\ d_G(u, v), & \text{otherwise.} \end{cases}$$

From the definition of Harary matrix, we know that

$$\begin{aligned} \rho(G'') - \rho(G) &\geq X^T R D(G'') X - X^T R D(G) X \\ &= \sum_{u, v \in V(G)} \left(\frac{1}{d_{G''}(u, v)} - \frac{1}{d_G(u, v)} \right) x_u x_v \\ &= 2 \sum_{u \in R_2, v \notin R_2} \left(\frac{1}{d_{G''}(u, v)} - \frac{1}{d_G(u, v)} \right) x_u x_v \\ &= 2r_2 a_2 \left(\sum_{v \in R_1} \left(\frac{1}{2} - \frac{1}{3} \right) x_v + \left(1 - \frac{1}{2} \right) x_{v_1} + \left(\frac{1}{2} - 1 \right) x_{v_2} \right) \\ &= \frac{1}{3} r_1 r_2 a_1 a_2 + r_2 a_2 (x_{v_1} - x_{v_2}) \\ &> 0. \end{aligned}$$

By repeating this process until all the pendant edges have a common end, we can obtain our conclusion. \square

From Lemma 2.1, Lemma 5.1 and Lemma 5.2, we have the following theorem.

Theorem 5.3. *Let G be a graph on n vertices with p cut edges which has the maximum Harary spectral radius, then $G = K_{n-p}(p)$.*

Corollary 5.4. *The n -vertex star S_n is the unique tree on n vertices which has the maximum Harary spectral radius.*

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